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TESTING OF ENDF/B-VIII.0 IN THE GNDS FORMAT WITH LLNL TRANSPORT CODES

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ENDF/B-VIII.0 was released in the Evaluated Nuclear Data Format and the Generalized Nuclear Data Structure format (GNDS), a new international standard for storing nuclear data developed under the auspices of the Nuclear Energy Agency Working Party on Evaluation Cooperation Subgroup 38. GNDS relies on modern coding practices, and offers a structured, flexible and physics-based standard for storing and exchanging nuclear data to address limitations in legacy nuclear data formats such as ENDF-6. GNDS supports the storage of evaluated nuclear data as well as processed data suitable for both deterministic (i.e., multi-group) and Monte Carlo transport codes. Lawrence Livermore National Laboratory has implemented a complete suite of codes to test GNDS data. Simulations for the ENDF/B-VIII.0 cross-section library in GNDS format are presented. Deterministic and Monte Carlo radiation transport simulations with the Ardra and Mercury codes respectively, are validated against reactivities in fast criticality safety benchmark assemblies. Finally, Mercury simulations of $^{238}U(n,f)$, $^{237}Np(n,f)$ *and* $^{239}Pu(n,f)$ *reaction rates in Godiva, Jezebel and Flattop are compared to MCNP results and measured data.*

I. INTRODUCTION

ENDF/B-VIII.0, the latest version of the US Evaluated Nuclear Data Library, was released in both the Evaluated Nuclear Data Format (ENDF-6)[1] and the Generalized Nuclear Data Structure[2, 3] (GNDS) format. GNDS is a new international standard for storing nuclear data. It was developed to address limitations in current nuclear data formats, such as ENDF-6[1], by offering a structured, flexible and physics-based standard for storing and exchanging evaluated and processed nuclear data.

Many institutions have tools to perform extensive testing of ENDF-6 formatted data. Currently, only Lawrence Livermore National Laboratory (LLNL) has the array of codes necessary to test GNDS formatted data. Testing of GNDS data has three major steps. Firstly, the nuclear data in ENDF-6 format are translated into the GNDS format if needed. Secondly, the GNDS formatted data are processed to add derived data necessary for transport codes (e.g., multi-group cross sections). Thirdly, transport codes read the GNDS formatted data, and simulate a particle transport system. LLNL updated the FUDGE (For Updating Data and Generating Evaluations) infrastructure to handle the translation and processing steps, and a low-level C++ API dubbed GIDI[4] (Generalized Interaction Data Interface) to allow transport codes to access GNDS data. GIDI was implemented in ARDRA[5,6] and Mercury[7], LLNL general-purpose deterministic and Monte Carlo radiation transport codes respectively. To test cross-section libraries, LLNL has developed a verification and validation (V&V) test suite that consists of ARDRA and Mercury models of fast criticality benchmark experiments from the handbook of International Criticality Safety Benchmark Evaluation Project (ICSBEP)[8], as well as activation and pulsed sphere experiments. This test suite was used to test ENDF/B-VIII.0/GNDS data.

The following sections give an overview of the GNDS format, describe the FUDGE code package, the GIDI and MCGIDI APIs, and the LLNL transport codes, and LLNL automated test suite. In the last section, simulations of integral benchmark experiments with the ENDFB-VIII.0 cross section library in the GNDS format are compared to MCNP results.

II. GENERALIZED NUCLEAR DATA STRUCTURE

The Generalized Nuclear Data structure is a new international standard for storing nuclear data. The standard was designed by WPEC sub-group 38: an international collaboration organized under the Working Party for Evaluation Co-operation (WPEC). GNDS is more flexible than previous standards, and able to store both evaluated and processed data in the same hierarchy. GNDS defines the structure for storing reaction data for a **PRO**jectile hitting a **TAR**get for a specified **E**valuation (e.g., ENDF/B-VII.1, ENDF/B-VIII.0). This combination is sometimes called a 'PROTARE'. Each protare contains information about all relevant reactions evaluated for that projectile and target. A single GNDS file (i.e., protare file) can simultaneously contain cross sections at various material temperatures and data for various multi-group structures.

Another new data hierarchy called Properties of Particles (or PoPs) has been developed along with GNDS. PoPs stores reaction-independent particle properties such as mass, spin and parity, half-life and decay properties. GNDS evaluations contain and/or link to a PoPs database.

III. FUDGE TRANSLATION/PROCESSING CODE

FUDGE is the principal code used by LLNL for managing and processing nuclear data. The code is written in Python with extensions in C and C++ to handle computation-intensive tasks. While originally written to handle LLNL's legacy Evaluated Nuclear Data Library (ENDL) format, FUDGE has been expanded to support GNDS. In addition to data processing, the code includes translators for converting data in ENDL and ENDF-6 formats into GNDS, as well as converting GNDS back to ENDF-6. Finally, a new functionality has been developed in FUDGE to translate GNDS data into MCNP ACE files to facilitate data and code comparison,

FUDGE contains many operations for processing data for use in transport simulations including:

- If applicable, reconstructing pointwise cross sections from resonance parameters. Special treatment for the unresolved resonance region (i.e. probability tables or Bondarenko factors) are not yet implemented in FUDGE.
- Doppler-broadening cross sections to account for material temperature.
- Putting cross sections on a common energy grid (for more efficient sampling during Monte Carlo transport) and generating cumulative probability density functions (CDFs) for outgoing energy/angle distributions.
- Generating flux-weighted multi-group cross sections and transfer matrices by integrating over incident energy, outgoing energy and angle. FUDGE acts as a wrapper for a new C++ code, Merced, which generates multigroup transfer matrices for deterministic transport.

After each operation, results can be stored back in GNDS along with a label indicating what style (i.e., operation) of data they are associated with. To simplify data processing, FUDGE includes a script called 'processProtare.py' which processes a single GNDS file. The script has command-line options for selecting what types of data to generate (e.g., temperature of the material, continuous energy for Monte Carlo, multi-group).

A regression test suite for FUDGE and GNDS has been developed and is used to improve the development cycle and provide quality assurance.

IV. GIDI/MCGIDI

The General Interaction Data Interface (GIDI) is a C++ API code developed at LLNL that enables reading GNDS data into transport codes. GIDI has classes corresponding to each level in the GNDS data hierarchy, including the Protare and Map classes. The Protare class reads data in from a single GNDS file which contains data for a protare. The Map class reads in a map file which contains a library of GNDS files and/or other map files. In a map file, each GNDS file is specified by its projectile, target, evaluation and file path. To read in a GNDS file, a user specifies a map file, and the desired projectile, target and evaluation. In general, the GIDI classes mimic the GNDS. For example, a Protare instance contains the list of reactions as Reaction class instances. The total multi-group cross section can be obtained by calling the crossSection method of a Protare instance. The cross section for a reaction can be obtained by calling the crossSection method for that Reaction instance. The crossSection methods take an argument which is used to specify which multi-group data are being requested (recall that a single GNDS can contain multiple temperature/multi-grouped data) and how the multi-group cross-section should be collapsed (i.e., reduced to a smaller set of groups).

GIDI contains the functionality to access all data needed for both deterministic and Monte Carlo transport from a GNDS file. It also supports some data processing steps, such as collapsing multi-group data down to a smaller set of groups. Practically, GIDI uses Properties of Particles (PoPs), alias and map files to define particle properties (e.g., masses, half-lives), particle aliases (e.g., '8016' for 'O16'), and to combine in one location information on available protares.

MCGIDI is a C++ code developed specifically for Monte Carlo transport codes to evaluate (e.g., obtain the cross section at an incident energy) and sample from GNDS data. Like GIDI, MCGIDI has a Protare class. This class takes a GIDI Protare as an argument as well as other arguments that describe what data to extract from the GIDI Protare. The extracted data are put into a form adapted to Monte Carlo transport. MCGIDI has two main types of methods that:

- sample a reaction in a Protare instance and sample outgoing particles for a given reaction.
- serialize MCGIDI data for MPI broadcasting and for copying to GPUs. It runs on "traditional" CPU as well as on GPUs.

The regression test suite developed for FUDGE quality assurance will also be extended to cover core capabilities in the GIDI and MCGIDI APIs. It can be extended to include performance testing as well as integration/acceptance testing for use with transport codes such as Mercury and Ardra described in the next section.

V. TRANSPORT CODES

V.A. Mercury

Mercury is a general-purpose Monte Carlo radiation transport code developed at LLNL. It was originally designed to use LLNL's Monte Carlo All Particles Transport (MCAPM) library to access nuclear data processed from LLNL Evaluated Nuclear Data Library (ENDL) format and to sample from reactions involving neutron, gammas and light charged particles [6]. Mercury handles energy either as continuous energy, fixed grid, or multigroup, where the multigroup mode is only for specific cross-section and multiplicity lookups. Collisions are handled as continuous energy. It is a massively parallel transport code that has scaled to all of the Sequoia machine, LLNL's BG/Q architecture. Mercury has recently been modified with a command-line option to allow switching between using MCAPM and GIDI/MCGIDI to read and sample nuclear data. MCAPM will eventually be deprecated and the GNDS/GIDI nuclear data capability will be the sole version available in Mercury.

V.B Ardra

Ardra is a general-purpose, massively parallel, discrete-ordinates (S_N) radiation transport code developed at LLNL. Ardra solves the linear Boltzmann transport equation for neutron and gamma transport across a wide range of problems including criticality, shielding, and source-detector problems[5,6]. Ardra has the ability to read multigroup nuclear data libraries, including ENDL via the ndf interface and GNDS via the GIDI interface. The NDI interface was also implemented in Ardra to read in data processed with NJOY. The GNDS/GIDI nuclear data capability will become Ardra's default once it is fully tested.

VI. AUTOMATED TEST SUITE

The LLNL Validation and Verification test suite was designed to be modular and easy to use. It includes python scripts and input files that allow to generate and query a database of input files, to run a selected set of problems and to compare results to simulations or benchmarks.

Three types of benchmark experiments are modeled: fast criticality experiments taken from the handbook of International Criticality Safety Benchmark Evaluation Project (ICSBEP)[7], as well as activation experiments and LLNL pulsed sphere experiments. Mercury tests include 123 critical assemblies, 5 activation experiments and 16 pulsed spheres, while Ardra tests consists of 1D problems, 79 critical assemblies and 4 activation experiments. Outputs consists of k_{eff}, reactions rates, and time-of-flight spectra. Once simulations are completed, results are compared and reported as Pass/Fail according to user-defined criteria. Plots and summary tables are also provided. In addition to Ardra and Mercury, the suite was expanded to include a set of MCNP[10] and COG[11] criticality benchmarks.

The test suite has demonstrated the ability to offer a fast turn-around solution when testing new evaluations or new release candidates of a nuclear data library. Simulations are run on a Livermore Computing (LC) system with 2,688 nodes, 36 cores per nodes and 343 TB of memory. Results can be obtained within 24 hours from data translation and processing to the completion of all Monte Carlo simulations. These run on 8 nodes while the S_n simulations are completed within 2 hours and typically run on 1 node.

VII. RESULTS

The ENDF/B-VIII.0 cross section library was translated from ENDF-6 to GNDS format and processed with the FUDGE code package. The processed library was then tested with Mercury and Ardra 1D models of fast benchmark critical assemblies. In addition, activation experiments in Godiva, Jezebel and Flattop25 were simulated with Mercury. Monte Carlo simulations were run using continuous energy (CE) cross-sections while Ardra simulations used multigroup cross-sections processed in 230 energy groups. The precision of Ardra deterministic calculations was 1e-6. Mercury Monte Carlo criticality calculations were run with 1e+6 neutron histories per cycle, 30 initial cycles to settle the neutron source and a maximum of 5000 iterations to achieve a convergence criterion of 1e-4 for the fractional standard deviation.

VII.A Criticality benchmarks

Ardra and Mercury eigenvalues for ENDF/B-VIII.0 are presented in Figure 1 for the suite of bare and reflected fast critical assemblies. Comparison to MCNP results calculated with ENDF/B-VIII.0 have been published elsewhere[13]. The benchmark k_{eff} ±1 standard deviation are plotted as gray lines. In general, Ardra simulations result in higher k effective than Mercury simulations. The largest discrepancies between the two codes are observed for critical assemblies with steel (Fe), Ni, Cu and Pb reflectors due to a limitation in the treatment of resonance self-shielding in Ardra that can be addressed by implementing the Bondarenko method for example. For both codes, reactivities of PU_MET_FAST_011, a water-reflected assembly, and PU_SOL_THERM_011, a solution assembly, differ from benchmarks by more than 2000 pcm. This is to be expected since neutrons thermal scattering laws are needed to simulate neutron transport in this type of assemblies and they still need to be implemented in FUDGE, GIDI and MCGIDI.

VII.B Reaction Ratios

While reaction rates are simulated routinely with the legacy version of Ardra using the ndf interface and with both versions of Mercury, it is currently being implemented in Ardra/GIDI and is not yet available for production runs.

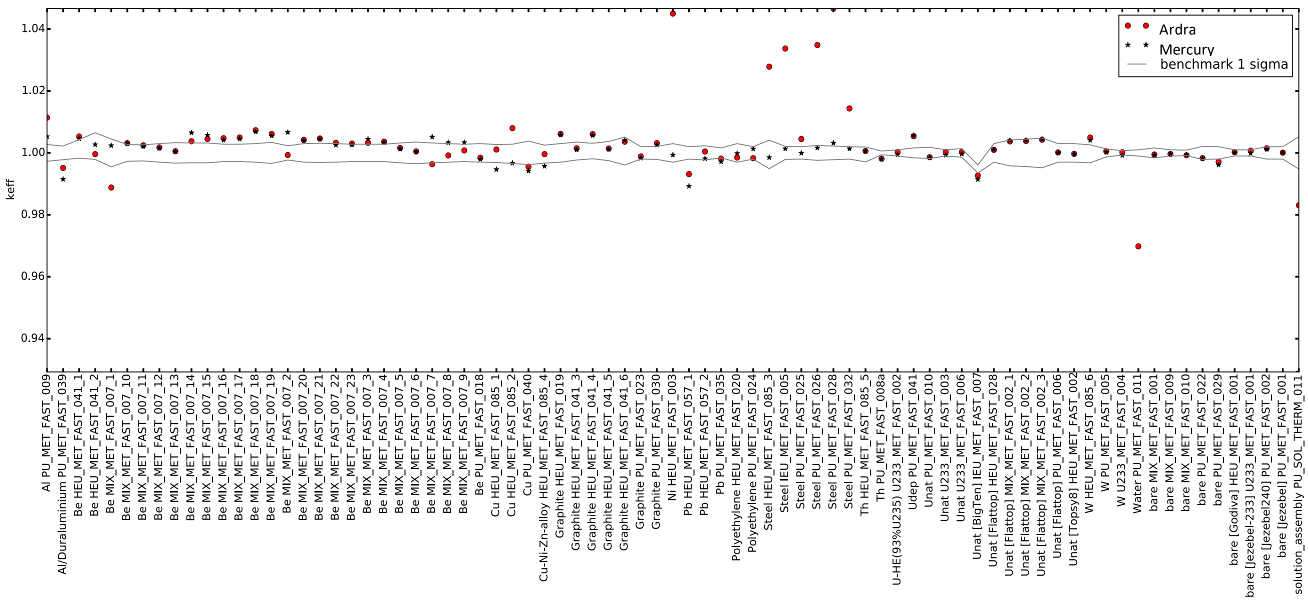

Figure 1. k effective for ICSBEP spherical criticality benchmarks ±1 standard deviation (black line) are compared to Ardra (red circle) and Mercury (black star) simulations using ENDF/B-VIII.0 in GNDS format. Cases are organized alphabetically by reflector material.

TABLE I. Comparison of reaction ratios for ENDF/B-VIII.0 calculated with Mercury (Merc) and MCNP and benchmark values measured in the center of three critical assemblies[9]. Results are normalized by ^{235}U(n,f).

Case	Code	^{238}U (n,f)	^{237}Np (n,f)	^{239}Pu (n,f)
Godiva	Merc.	0.1583	0.8314	1.3844
	MCNP	0.1583	0.8318	1.3846
	Exp. w/	0.1643	0.8516	1.4152
	uncertainty	0.0018	0.012	0.014
	Merc/MCNP	1.0001	0.9995	0.9998
	Merc/Exp.	0.9635	0.9763	0.9782
Jezebel	Merc.	0.2120	0.9772	1.4275
	MCNP	0.2121	0.9770	1.4273
	Exp. w/	0.2133	0.9835	1.4609
	uncertainty	0.0023	0.014	0.013
	Merc/MCNP	0.9997	1.0002	1.0001
	Merc/Exp.	0.9939	0.9936	0.9771
Flattop 25	Merc.	0.1450	0.7737	1.3621
	MCNP	0.1451	0.7735	1.3622
	Exp. w/	0.1492	0.7804	1.3847
	uncertainty	0.0016	0.01	0.012
	Merc/MCNP	0.9990	1.0003	0.9999
	Merc/Exp.	0.9718	0.9914	0.9837

Reaction rates for ^{238}U(n,f), ^{237}Np(n,f), and ^{239}Pu(n,f) in a small spherical region at the center of the Godiva, Jezebel and Flattop25 assemblies were simulated with Mercury. Results are normalized by the ^{235}U(n,f) reaction rate for each assembly and are compared to MCNP simulations and to measured data from foil activation experiments. They are presented in Table 1. There is excellent agreement with MNCP reaction ratios published in the ENDF/B-VIII.0 reference article[9] and relatively good agreement with experimental data.

VII. CONCLUSION AND FUTURE WORK

The ENDF/B-VIII.0 nuclear data library was recently released in the ENDF-6 and GNDS format, a new international standard for storing nuclear data designed by WPEC sub-group 38. Over the past few years, LLNL has developed a complete array of codes to process and test GNDS formatted data including the FUDGE code package to translate and process the GNDS data, and the GIDI and MCGIDI APIs implemented in Mercury and Ardra, LLNL's Monte Carlo and deterministic transport codes.

The ENDF/B-VIII.0 neutron sub-library was translated and processed with FUDGE. Ardra and Mercury simulations of integral benchmark experiments were compared to benchmark values. Reaction ratios in Godiva, Jezebel and Flattop25 were also compared to published MCNP results for ENDF/B-VIII.0. Overall, Mercury results show good agreement with MCNP and relatively good agreement with benchmark data.

While the results presented in the previous section demonstrate the LLNL suite of codes can successfully utilize nuclear data in GNDS format, several steps are needed to fully develop GNDS functionalities in these codes. Simulations of pulsed spheres experiments are ongoing to test the new angular biasing capability that was recently implemented in Mercury. Future work includes the implementation of neutron thermal scattering laws and the treatment of neutron cross sections in the unresolved resonance region (URR) in FUDGE, GIDI and MCGIDI. The test suite is being expanded to include thermal critical assemblies to test these capabilities once they are released. The current code suite can also handle photons and charged particles and we plan to develop testing capabilities accordingly.

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